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REEXAMINATION OF THE $O(^3P \rightarrow {}^1D)$ EXCITATION RATE BY THERMAL ELECTRON IMPACT

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Abstract: The theoretical and experimental electron impact excitation cross sections for the $O(^3P \rightarrow {}^1D)$ transition that have been reported in the literature the last two decades are used to derive $O(^3P \rightarrow {}^1D)$ excitation rates by thermal electron impact. The derived rates are represented by a simple parametric formula which should prove useful in atmospheric 6300-Å airglow and electron gas thermal balance studies.

Introduction

Excitation of the singlet D state of atomic oxygen, $O(^3P \rightarrow {}^1D)$, by thermal electron impact may contribute to the intensity of the 6300-Å line observed in the aurora and the dayglow. Indeed, thermal electron excitation of $O(^1D)$ is believed to be the primary source of mid-latitude stable aurora red (SAR) arcs and, under certain conditions, may also constitute the main source of the 6300-Å radiation observed in controlled ionosphere heating experiments.

In the past two decades, calculations of the contribution to the 6300-Å atmospheric radiation by thermal electron excitation of $O(^1D)$ have usually employed a rate coefficient derived by Rees et al., (1967) from a theoretically computed excitation cross section by Smith et al., (1967). This cross section was recalculated by Henry et al., (1969) to correct an error in the original theoretical formulation. For energies greater than 3 eV the corrected cross section is lower than the first by 25% - 35%. The correction makes little difference in the energy range 1.96 - 3 eV, which to a large extent determines the excitation rate for the electron temperatures found in the earth's ionosphere. Since then, additional calculations and measurements of the $O(^1D)$ electron impact excitation cross section have been reported. Link (1982) derived an excitation rate based on the Henry (1969) cross section, which has been employed in some subsequent work (e.g. Link et al, 1988; Solomon et al, 1988). To our knowledge, however, there has been no reassessment of the $O(^1D)$ thermal excitation rate coefficient in light of the progress in the theoretical and experimental results on the $O(^1D)$ excitation cross section. It is our purpose here to undertake this task.

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The $O(^3P \rightarrow {}^1D)$ Electron Impact Excitation Cross Section

In additional to the above, theoretical calculations of the $O(^1D)$ excitation cross section have been carried out by Vo Ky Lan et al., (1972) and by Thomas and Nesbet (1975). The results of Vo Ky Lan et al., (1972) are in close agreement with those of Henry et al., (1969), over the entire energy range. Those of Thomas and Nesbet, (1975), in the energy range 2 - 5 eV, are lower by a factor of nearly two. This is primarily because the excitation potential obtained by the authors for the $O(^1D)$ state is higher than the experimentally observed (by both energy loss and optical methods) and generally accepted value. A translation of their energy scale by -0.25 eV, would bring their results to closer agreement with those of Henry et al., (1969) and Vo Ky Lan et al., (1972).

In the laboratory, the $O(^1D)$ electron impact excitation cross section has been measured by Shyn and Sharp (1986) and, more recently, by Doering and Gulcicek (1989). The first of these experimental cross sections is in agreement with the theoretical results of Henry et al., (1969) and Vo Ky Lan et al., (1972) over the entire energy range (i.e., 7 - 30 eV) covered by the measurements. The second, while in agreement within experimental error with the aforementioned experimental and theoretical results at 30 eV, is increasingly higher at lower energies (nearly by a factor of 2 at 5 eV.)

A graphical representation of these cross sections, in the energy range 2 - 7 eV, is shown in Figure 1 (Points). In this energy interval, Figure 1 shows that the available theoretical and experimental cross sections are spread about their mean value from a few to over 50%.

The $O(^3P \rightarrow {}^1D)$ Thermal Electron Impact Excitation Rate

At an electron gas temperature of 2000 Kelvin only 0.01% of a maxwellian electron population has sufficient energy to excite the $O(^1D)$ state, which has an excitation threshold of 1.96 eV. At temperatures of 4000 and 6000 K, this fraction increases to 1.5% and 7.3%, respectively. Furthermore, at 6000 K only 0.15% of the electron population has energies greater than 4 eV. Therefore, for the range of temperatures encountered in the earth's ionosphere, i.e., 500 - 6000 Kelvin, the $O(^1D)$ excitation rate coefficient is largely determined by the magnitude of the cross section in an energy interval of a few eV width above the excitation threshold.

To obtain an analytic formula for the $O(^1D)$ thermal excitation rate it suffices therefore to adequately represent analytically the excitation

cross section in the energy range, say, 1.96 - 7 eV.

The formula

$$\sigma(E) = \sigma_0\ (E/W - 1)\ \mathrm{Exp}\{-(E - W)/(E_{max} - W)\}\ (\mathrm{cm}^2) \quad (1)$$

with W, E_{max}, and σ_0 as adjustable parameters, can adequately represent the cross section in this energy range and can be easily integrated over a maxwellian distribution. In (1) W is identified with the excitation threshold energy, 1.96 eV, E_{max} with the energy at which the cross section attains its maximum value and σ_0 can be determined by fitting (1) to the theoretical, or measured, cross section at any particular energy in the interval of interest, say, at $E = E_{max}$. Presently, in fitting (1) to the cross sections by Henry et al., (1969), Vo Ky Lan et al., (1972) and Doering and Gulcicek (1989) W was kept constant at 1.96 eV, while E_{max} and σ_0 were determined from a least squares fit in the energy range 1.96 - 7 eV. In the case of the cross section by Thomas and Nesbet (1975) all three parameters were allowed to vary in the least squares fit. The values of the parameters obtained in this manner are given in Table 1 (Part a) and the fitted curves are illustrated in Figure 1.

Integration of (1) over a maxwellian electron distribution and manipulation of the result leads to the expression

$$\alpha(T) = \alpha_0 \sqrt{T}\ \frac{(T_1 + T)}{(T_2 + T)^3}\ \mathrm{Exp}(-T_3/T)\ (\mathrm{cm}^3/\mathrm{sec}) \quad (2)$$

for the $O(^1D)$ thermal electron impact excitation rate, where: T is the electron gas temperature in Kelvin, and α_0, T_1, T_2, T_3 are constants (functions of the cross section fitting parameters, σ_0, E_{max} and W) whose values are given in Table 1 (Part b). A graphical representation of the thermal excitation rate, as given by (2), is shown in Figure 2.

The rate coefficients are compared in Figure 3, where we have plotted the ratio of each of the

Table 1. a) Values of the parameters (σ_0, E_{max}, W) for fitting Formula (1) to the $O(^1D)$ electron impact excitation cross section published by the indicated authors; b) coefficients (α_0, T_1, T_2, T_3) of the derived $O(^1D)$ thermal excitation rate (Formula 2). The cross sections are in cm^2 and the rate coefficient in $\mathrm{m}^3/\mathrm{sec}$.

σ_0	E_{max}	W	α_0	T_1	T_2	T_3	Cross Section by:
4.672E-17	5.133	1.960	0.167	8693	36840	22756	Henry et al., (1969)
5.145E-17	4.905	1.960	0.150	8537	34191	22756	Vo Ky Lan et al., (1972)
3.389E-17	6.934	2.216	0.332	10418	54779	25730	Thomas & Nesbet, (1975)
6.439E-17	6.423	1.960	0.596	9329	51813	22756	Doering & Gulcicek, (1989)

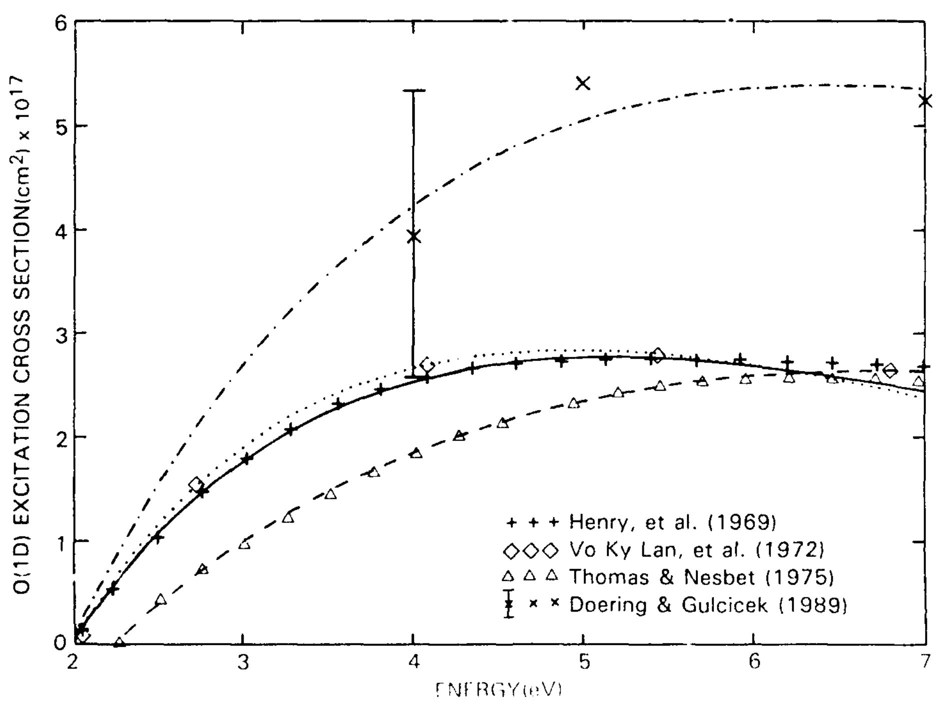

Fig. 1. Least squares fits (Curves) of Formula (1) to the electron impact $O(^1D)$ excitation cross sections. The fit parameters (σ_0, E_{max}, W) are given in Table 1.

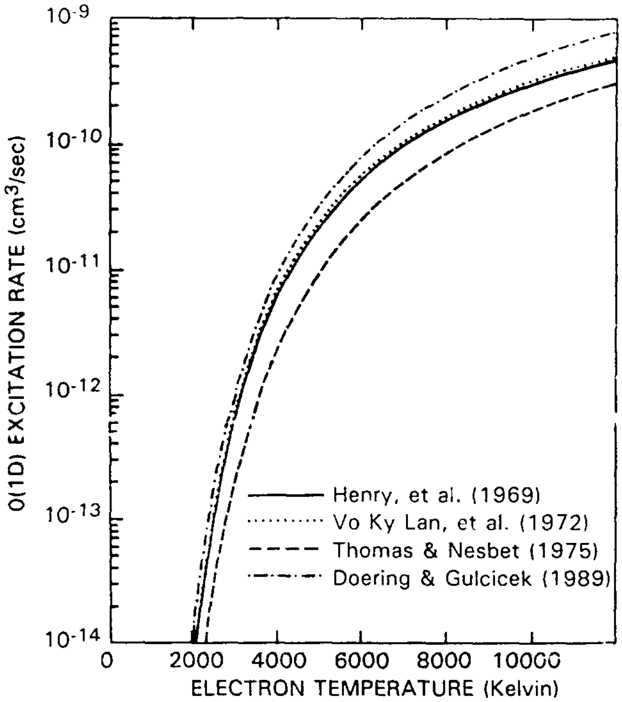

Fig. 2. Thermal electron impact excitation rates of $O(^1D)$. The coefficients (α_0, T_1, T_2, T_3) for Formula (2) are given in Table 1.

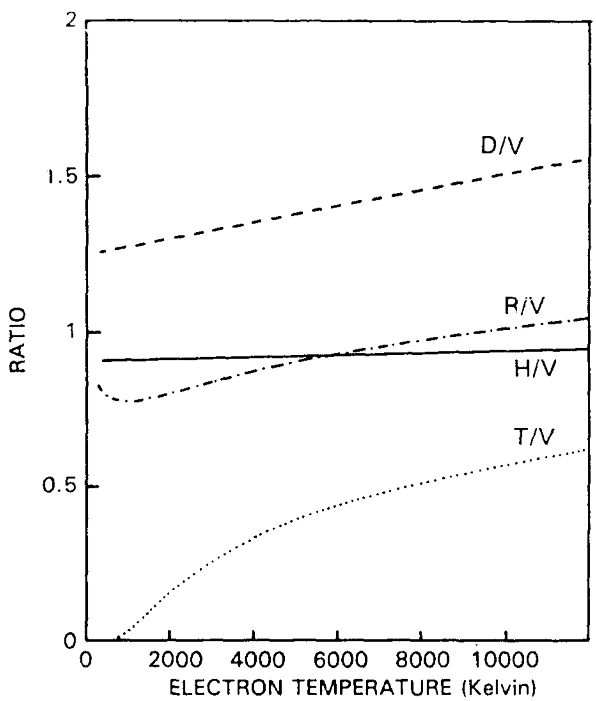

Fig. 3. Ratios of the thermal electron impact excitation rates of $O(^1D)$ corresponding to the cross section by Doering and Gulcicek (1989)[indicated by D/V], Henry et al., (1969)[indicated by H/V], and Thomas and Nesbet (1975)[indicated by T/V], with respect to the rate corresponding to the cross section by Vo Ky Lan et al., (1972). The ratio of the rate by Rees et al., (1967) is indicated by R/V.

computed rates to that derived from the cross section by Vo Ky Lan et al., (1972). In the same figure we have also plotted the ratio of the rate derived by Rees et al., (1967) from the cross section by Smith et al., (1967), since this rate has extensively been used in atmospheric 6300-Å airglow and electron gas thermal balance research. The figure shows that the rates deduced from the cross sections by Henry et al., (1969) and Vo Ky Lan et al., (1972) are in close agreement (differ only by 8% - 5% in the temperature range 350 to 12000 Kelvin.) The cross section by Doering and Gulcicek (1989) gives a rate coefficient higher by 25% - 55%, while that by Thomas and Nesbet (1975) gives a lower rate by >100% - 40%. The rate by Rees et al., differs from about -25% to +5%.

Discussion

The difficulties in reconciling observed and modeled 6300-Å airglow are well known (Hays et al., 1978; Cogger et al., 1980; Link and Cogger, 1988; Solomon et al., 1988; Solomon and Abreu, 1989). Hitherto, attention has been focused on better definition of photochemical sources, supra-thermal electron excitation, quenching rates, and transition probabilities. The difficulties that are inherent in an accurate determination of the $O(^1D)$ thermal electron excitation source, at least in cases where this source is significant, do not appear to have been adequately stressed. Apart from the uncertainty due to the inadequate knowledge of the cross section near the excitation threshold, Figure 2 shows that, due to the strong dependence of the thermal excitation rate on the electron gas temperature, a small uncertainty in the electron temperature leads to a large one in the excitation rate. For example, at an electron temperature of 2500 K an uncertainty of 5% in temperature leads to an uncertainty of 35% in the excitation rate. This uncertainty increases rapidly with decreasing temperature.

Conclusion

For the electron gas temperatures encountered in the earth's ionosphere, the derived thermal excitation rates $O(^3P\rightarrow^1D)$ are spread by order of 50% about their mean value, reflecting the differences in the excitation cross section reported in the literature. The theoretical cross section by Thomas and Nesbet (1975) gives the lowest rate, mainly due to the (unacceptably) high threshold potential reported in these calculations. The rates derived from the cross sections by Henry et al., (1969) and Vo Ky Lan et al., (1972) are for practical purposes almost identical. On theoretical grounds, the cross section calculations reported Vo Ky Lan et al., (1972) appear as the most complete of those presently available. The measurements of Shyn and Sharp (1986) support these results. However, they do not extend to energies below 7 eV and for this reason cannot be used for the present purpose. The rate based on the measured cross section by Doering and Gulcicek (1989) constitutes an upper bound of the present rates If supported by additional evidence, the significance of this result on the aeronomy of the 6300-Å radiation need not be here emphasized.

Presently, we recommend using the rate

$$\alpha(T) = 0.15\,\sqrt{T}\,\frac{(8537 + T)}{(34191 + T)^3}\,\mathrm{Exp}(-22756/T)\quad (\mathrm{cm}^3/\mathrm{sec}) \tag{3}$$

that is based on the cross section by Vo Ky Lan et al., (1972).

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